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## Abstract

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## 1. Introduction

Suppose  $X_1, \dots, X_n$  are i.i.d. from  $p$ -dimensional normal distribution  $N_p(\mu_X, \Sigma_X)$ . Denote  $X = (X_1, \dots, X_n)$ . In this paper, it is assumed that  $n < p$ , that is, high dimension setting is considered. Consider a linear regression model

$$y = \beta_0 \mathbf{1}_n + X^T \beta + \epsilon, \quad (1)$$

where  $\mathbf{1}_n$  is  $n$  dimensional vector with all elements equal to 1 and  $\epsilon$  has distribution  $N(0, \sigma^2 I_n)$ .

Let  $\Sigma_X = P \Lambda P^T$  be the spectral decomposition of  $\Sigma_X$ , where  $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_p)$  with  $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_p$  and  $P$  is an orthogonal matrix. In PCA context, it is assumed that  $\Sigma_X$  is spiked, that is  $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_r > \lambda_{r+1} = \dots = \lambda_p$  for some  $r > 0$  (See [1]). Denote by  $P_1$  the first  $r$  column of  $P$  and  $P_2$  the last  $p - r$  column of  $P$ . The aim of PCA is to estimate  $P_1$ . In this paper, we

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allow  $\Sigma_X$  to be either spiked or non-spiked. Non-spike means that there's no principal component ( $r = 0$ ). That is,  $\lambda_1 = \dots = \lambda_p$ . Spike means that there's  $r$  principal components for  $r > 0$ . In either case, let  $\lambda = \lambda_{r+1} = \dots = \lambda_p$ .

If  $\Sigma_X$  is indeed spiked,

$$y = \beta_0 \mathbf{1}_n + X^T P_1 P_1^T \beta + X^T P_2 P_2^T \beta + \epsilon, \quad (2)$$

where  $X^T P_1$  and  $X^T P_2$  are independent. PCR try to do regression between  $y$  and  $X^T P_1$ . Since  $P_1$  is not observed, it is substituted by an estimator  $\tilde{P}_1$ . Traditionally, PCR is a technique for analyzing multiple regression data that suffers from multicollinearity. Recently, PCR is a practical method to deal with high dimensional regression. If  $p < n$ , the full multicollinearity phenomenon shows up even if predictors are independent. It calls for a test procedure to justify the appropriateness of PCR. To be precise, we consider testing the hypotheses

$$H : \Sigma \text{ is non-spiked or } \Sigma \text{ is spiked and } P_1^T \beta = 0 \quad (3)$$

versus

$$K : \Sigma \text{ is spiked and } P_1^T \beta \neq 0. \quad (4)$$

If  $P_1$  is observed, then the problem is reduced to testing an ordinary regression model. However, it's not the case. In fact, the classical  $F$ -test statistic for the regression between  $y$  and  $X^T \tilde{P}_1$  may not be a good choice for at least three reasons:

1. From equation

$$y = \beta_0 \mathbf{1}_n + X^T \tilde{P}_1 \tilde{P}_1^T \beta + X^T (I_p - \tilde{P}_1 \tilde{P}_1^T) \beta + \epsilon, \quad (5)$$

we can see that the  $F$ -test suffers from Endogeneity.

2. The estimator of  $P_1$  may not be consistent in high dimension. Moreover,  $\Sigma_X$  may not be spiked and, as a result, there's no principal component.
3. Even if there's additional information or data to estimate  $P_1$ , we will never know weather we estimate  $P_1$  well enough such that the  $F$ -test is valid.

[2] proposed a generalized likelihood ratio test (GLRT) for testing high dimensional mean values. Roughly speaking, GLRT projects data to lower dimension by a direction  $a$  such that likelihood ratio is maximized. GLRT is likelihood based, it can be regarded as a generalization of classical LRT in high dimension setting.

In this paper we apply the GLRT method to the problem of testing the significance of PCR.

## 2. New Test

It can be seen that  $(X_1^T, y_1)^T, \dots, (X_n^T, y_n)^T$  are i.i.d. from  $N_{p+1}(\mu, \Sigma)$ , where  $\mu = (\mu_X^T, \beta_0)^T$  and

$$\Sigma = \begin{pmatrix} \Sigma_X & \Sigma_X \beta \\ \beta^T \Sigma_X & \beta^T \Sigma_X \beta + \sigma^2 \end{pmatrix}. \quad (6)$$

Denote  $\Theta : (\mu, \Sigma)$ . Define the hypothesis  $H_a$  by

$$H_a : \text{Cov}(a^T X_i, y_i) = 0, \quad (7)$$

where  $a \in \mathbb{R}^p$  and  $a^T a = 1$ . Let

$$S = \frac{1}{n} \sum_{i=1}^n \begin{pmatrix} (X_i - \bar{X})(X_i - \bar{X})^T & (X_i - \bar{X})(y_i - \bar{y})^T \\ (y_i - \bar{y})(X_i - \bar{X})^T & (y_i - \bar{y})(y_i - \bar{y})^T \end{pmatrix} = \begin{pmatrix} S_{XX} & S_{XY} \\ S_{YX} & S_{YY} \end{pmatrix}, \quad (8)$$

and

$$S_a = \begin{pmatrix} a^T & 0 \\ 0 & 1 \end{pmatrix} S \begin{pmatrix} a & 0 \\ 0 & 1 \end{pmatrix}, \Sigma_a = \begin{pmatrix} a^T & 0 \\ 0 & 1 \end{pmatrix} \Sigma \begin{pmatrix} a & 0 \\ 0 & 1 \end{pmatrix}. \quad (9)$$

The likelihood function of  $(a^T X_i, y_i)$ ,  $i = 1, \dots, n$ , is

$$L_a(\theta; X, Y) = (2\pi)^{-n} |\Sigma_a|^{-n/2} \exp\left(-\frac{1}{2} \text{tr} \Sigma_a^{-1} S_a\right). \quad (10)$$

Then the maximum likelihood is

$$L(a) = \sup_{\theta \in \Theta} L_a(\theta; X, Y) = (2\pi)^{-n} |S_a|^{-n/2} e^{-n}. \quad (11)$$

If  $|S_a| = 0$ , then 11 is interpreted as  $+\infty$ . Similarly, the maximum likelihood under  $H_a$  is

$$L(a) = \sup_{\theta \in H} L_a(\theta; X, Y) = (2\pi)^{-n} |a^T S_{XX} a S_{yy}|^{-n/2} e^{-n}. \quad (12)$$

In [2], GLRT is defined as

$$\min_{L(a)=+\infty} L_H(a) \quad s.t. \quad a^T a = 1. \quad (13)$$

The idea of GLRT is to find  $a$  such that  $L(a) = +\infty$  and  $L_H(a) < +\infty$  as small as possible such that the discrepancy between the likelihood values  $L(a)$  and  $L_H(a)$  is maximized. We call the direction  $a^*$  obtained by (13) the GLRT direction.

From the expression of  $L(a)$  and  $L_H(a)$ ,  $a^*$  is equal to

$$a^* = \operatorname{argmax}_{a^T a = 1} a^T S_{XX} a \quad s.t. \quad |S_a| = 0. \quad (14)$$

Such a direction  $a^*$  can be expected to make  $|\Sigma_a|$  small and  $a^T \Sigma_{XX} a$  large. That is, the variance of  $a^T X_i$  is large and  $a^T X_i$  and  $y_i$  are highly correlated. If  $X_i$  has certain principal components which are correlated to  $y_i$ , the direction  $a^*$  is expected to be close to corresponding principal directions.

Next we solve the optimization problem (14). Let  $Q_n = I_n - \frac{1}{n} \mathbf{1}_n \mathbf{1}_n^T$ . Denote by  $Q_n = W W^T$  the rank decomposition of  $Q_n$ , where  $W_n$  is an  $n \times (n-1)$  matrix with  $W^T W = I_{n-1}$ . Then  $|S_a| = 0$  is equivalent to  $a^T X Q X^T a y^T Q y = (a^T X Q y)^2$  and is equivalent to  $W^T X^T a = W^T y k$  for some  $k \in \mathbb{R}$ . It follows that

$$a = X W (W^T X^T X W)^{-1} W^T y k + (I - X W (W^T X^T X W)^{-1} W^T X^T) a. \quad (15)$$

Since  $a^T a = 1$ ,

$$k^2 y^T W (W^T X^T X W)^{-1} W^T y + a^T (I - X W (W^T X^T X W)^{-1} W^T X^T) a = 1. \quad (16)$$

Note that

$$L_H(a) \propto (a^T X Q X^T a y^T Q y)^{-n/2} = (k^2 (y^T Q_n y)^2)^{-n/2}. \quad (17)$$

To make  $L_H(a)$  minimized, we should maximize  $k^2$ . So the second term of 16 should be 0. That is

$$a = XW(W^T X^T XW)^{-1} W^T y k \quad (18)$$

Hence

$$k^2 = \frac{1}{y^T W(W^T X^T XW)^{-1} W^T y}, \quad (19)$$

and

$$L_H(a) \propto (a^T X Q X^T a y^T Q y)^{-n/2} = \left( \frac{(y^T Q_n y)^2}{y^T W(W^T X^T XW)^{-1} W^T y} \right)^{-n/2}. \quad (20)$$

After homogenization, we define

$$T = \frac{y^T Q_n y}{y^T W(W^T X^T XW)^{-1} W^T y}.$$

If  $T$  is large, we reject  $H$ .

### 3. Main Results

Let  $\tilde{y} = W^T y$ ,  $\tilde{X} = XW$ ,  $\tilde{\epsilon} = W^T \epsilon$ . Then the columns of  $\tilde{X}$  are i.i.d. distributed as  $N(0, \Sigma_X)$ ,  $\tilde{\epsilon} \sim N(0, \sigma^2 I_{n-1})$  and  $\tilde{y} = \tilde{X}^T \beta + \tilde{\epsilon}$ . The test statistic can be written as

$$T = \frac{\tilde{y}^T \tilde{y}}{\tilde{y}^T (\tilde{X}^T \tilde{X})^{-1} \tilde{y}}.$$

We make the following assumption.

**Assumption 1.** Assume model (1) holds with the columns of  $X$  i.i.d. distributed as  $N(\mu_X, \Sigma_X)$ ,  $\epsilon \sim N(0, \sigma^2 I_n)$  and  $\sigma^2$  is fixed as  $n, p \rightarrow \infty$ .

**Assumption 2.** Assume the eigenvalues of  $\Sigma_X$  satisfy  $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_r > \lambda_{r+1} = \dots = \lambda_p = \lambda$ , where  $r \geq 0$  and  $\lambda > 0$  are fixed as  $n, p \rightarrow \infty$ ,  $\lambda_1 \asymp \lambda_r$  and  $p^{1/2}/\lambda_r \rightarrow 0$ . We say there's no principal component if  $r = 0$ , that is  $\lambda_1 = \dots = \lambda_p$ .

The null hypotheses  $H$  is the union of two disjoint hypothesis  $H = \cup_{i=1}^2 H_i$ , where  $H_1$ : There's no principal component; and  $H_2$ : There's  $r$  principal components with  $r > 0$  and  $P_1^T \beta = 0$ . Under  $H_1$  we have the following theorem

**Theorem 1.** Suppose Assumptions 1 and 2 hold. Assume  $p/n \rightarrow \infty$  and  $H_1$  is true. Then

$$T/(\lambda p) \xrightarrow{P} 1. \quad (21)$$

If  $\|\beta\|^2 = o(\frac{n}{p})$  or  $\|\beta\|^{-2} = o(\frac{n}{p})$ , then for  $\alpha \in (0, 1)$  we have

$$\Pr \left( \frac{T - \lambda p}{\lambda \sqrt{2p}} \geq \Phi^{-1}(1 - \alpha) \right) \leq \alpha. \quad (22)$$

**Remark 1.** It can be seen from our proof that if  $\|\beta\|^2 = o(\frac{n}{p})$  and  $\|\beta\|^{-2} = o(\frac{n}{p})$  are both fail, then the asymptotic property of  $T$  is sophisticated.

Under  $H_2$  we have a similar theorem with one more condition  $p = o(n^2)$ .

**Theorem 2.** Suppose Assumptions 1 and 2 hold. Assume  $p/n \rightarrow \infty$ ,  $p/n^2 \rightarrow 0$  and  $H_2$  is true. Then

$$T/(\lambda p) \xrightarrow{P} 1. \quad (23)$$

If  $\|P_2^T \beta\|^2 = o(\frac{n}{p})$  or  $\|P_2^T \beta\|^{-2} = o(\frac{n}{p})$ , then for  $\alpha \in (0, 1)$  we have

$$\Pr \left( \frac{T - \lambda p}{\lambda \sqrt{2p}} \geq \Phi^{-1}(1 - \alpha) \right) \leq \alpha. \quad (24)$$

Under  $K$ , to simplify the proof, we assume  $\beta$  is generated from a normal prior distribution before data are generated. Denote by  $\Phi(\cdot)$  the CDF of normal distribution. We have the following theorem:

**Theorem 3.** Suppose Assumptions 1 and 2 hold. Assume  $p/n \rightarrow \infty$  and  $K$  is true. Assume  $\beta$  has prior distribution  $N(0, \sigma_\beta^2 I_p)$ . Assume that

$$\frac{np^2 + p^{5/2} + \lambda_1 p^{3/2}}{(p + \lambda_1)^2} \sigma_\beta^2 \rightarrow \infty, \quad (25)$$

then

$$\Pr \left( \frac{T - p\lambda}{\lambda \sqrt{2p}} \geq \Phi^{-1}(1 - \alpha) \right) = E\Phi \left( -\Phi^{-1}(1 - \alpha) + \frac{\sum_{i=1}^r \lambda_i \chi_i^2}{\lambda \sqrt{2p}} \right) + o(1). \quad (26)$$

**Remark 2.** If  $\lambda_1/\sqrt{p} \rightarrow \infty$ , then

$$\Pr \left( \frac{T - p\lambda}{\lambda \sqrt{2p}} \geq \Phi^{-1}(1 - \alpha) \right) \rightarrow 1. \quad (27)$$

Since  $\lambda$  is unknown, an estimator should be substituted. A natural estimator is

$$\frac{1}{(p-r)(n-1)} \sum_{i=r+1}^{n-1} \lambda_i(\tilde{X}^T \tilde{X}). \quad (28)$$

However,  $r$  is unknown, which itself need to be estimated consistently. If  $r > 0$ , it can be well estimated (See [3]). However, if  $r = 0$ , which may occur in our problem, the method in [3] fails. Nevertheless, it's easy to find an estimator which is not less than  $r$ . In following theorem, we will assume  $k$  is a fixed number such that  $k \geq r$ .

**Theorem 4.** *Suppose Assumptions 1 and 2 hold. Assume  $p/n \rightarrow \infty$  and  $k \geq r$  is a fixed integer. Let*

$$\frac{1}{(p-k)(n-1)} \sum_{i=k+1}^{n-1} \lambda_i(\tilde{X}^T \tilde{X}). \quad (29)$$

*Then*

$$\hat{\lambda} = \lambda + O_P\left(\frac{1}{n}\right). \quad (30)$$

*Furthermore, if we add condition  $p = o(n^2)$  to Theorem 1, add condition  $(p + \lambda_1)/(n\sqrt{p}) \rightarrow 0$  to Theorem 3, then the conclusion of Theorem 1, 2 and 3 holds with  $\lambda$  substituted by  $\hat{\lambda}$ .*

**Remark 3.** It is not hard to generalize our results for a random positive integer  $k$  such that  $\Pr(k \geq r) \rightarrow 1$  and  $k \leq M$  for some  $M > 0$ .

**Remark 4.** In practice,  $r$  is often small. Hence it's often the case that we could choose a known upper bound for  $r$ .

By our theoretic results, we reject the hypotheses when

$$\frac{T - p\lambda}{\lambda\sqrt{2p}} \geq \Phi^{-1}(1 - \alpha). \quad (31)$$

Under the condition of Theorem 1 and Theorem 2, the test level can be guaranteed. The test power is given by Theorem 3.

#### 4. Appendix

For random variables  $\xi$  and  $\eta$ , we write  $\xi \sim \eta$  when  $\xi$  and  $\eta$  have the same distribution. For two sequences of positive random variables  $\xi_n$  and  $\eta_n$ , we write  $\xi_n \asymp \eta_n$  if  $\Pr(c\eta_n \leq \xi_n \leq C\eta_n) \rightarrow 1$  for some positive  $c$  and  $C$ .

$$\begin{aligned} T &= \frac{\beta^T \tilde{X} \tilde{X}^T \beta + 2\beta^T \tilde{X} \tilde{\epsilon} + \tilde{\epsilon}^T \tilde{\epsilon}}{\beta^T \tilde{X} (\tilde{X}^T \tilde{X})^{-1} \tilde{X}^T \beta + 2\beta^T \tilde{X} (\tilde{X}^T \tilde{X})^{-1} \tilde{\epsilon} + \tilde{\epsilon}^T (\tilde{X}^T \tilde{X})^{-1} \tilde{\epsilon}} \\ &= \frac{A_1 + A_2 + A_3}{B_1 + B_2 + B_3}. \end{aligned} \quad (32)$$

##### 4.1. Lemma

**Lemma 1.** Suppose  $A$  is an  $n \times n$  full rank symmetric matrix. And let

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}, \quad (33)$$

where  $A_{11}$  is a real number,  $A_{12}$  is a  $1 \times (n-1)$  matrix,  $A_{21}$  is a  $(n-1) \times 1$  matrix and  $A_{22}$  is a  $(n-1) \times (n-1)$  matrix. Denote  $A_{11.2} = A_{11} - A_{12} A_{22}^{-1} A_{21}$ . Then we have

$$(A^{-1})_{11} = A_{11.2}^{-1} \quad (34)$$

**Lemma 2.** Let  $H$  and  $P$  be two symmetric matrices and  $M = H + P$ . If  $j + k - n \geq i \geq r + s - 1$ , we have

$$\lambda_j(H) + \lambda_k(P) \leq \lambda_i(M) \leq \lambda_r(H) + \lambda_s(P). \quad (35)$$

Lemma 2 is known as the Weyl's inequality.

**Lemma 3.** Suppose  $B = \frac{1}{q} V V^T$  where  $V$  is an  $p \times q$  random matrix composed of i.i.d. random variables with zero mean, unit variance and finite fourth moment. As  $q \rightarrow \infty$  and  $p/q \rightarrow c \in [0, +\infty)$ , the largest and smallest nonzero eigenvalues of  $B$  converge almost surely to  $(1 + \sqrt{c})^2$  and  $(1 - \sqrt{c})^2$ , respectively.

Lemma 3 is known as the Bai-Yin's law [4].



**Lemma 4.** Let  $Z_1, \dots, Z_{n+1}$  i.i.d. distributed as  $N(0, I_p)$ .  $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_p)$ , where  $\lambda_1 \geq \dots \geq \lambda_r$  and  $\lambda_{r+1} = \dots = \lambda_p = \lambda$ .  $\limsup_{n \rightarrow \infty} \lambda_1 / \lambda_r < \infty$ ,  $\lambda_1 / \sqrt{p} \rightarrow \infty$ . Suppose  $p = o(n^2)$ . Denote  $Z = (Z_1, \dots, Z_n)$ . Let  $\hat{V}$  be the first  $r$  eigenvectors of  $\Lambda^{1/2} Z Z^T \Lambda^{1/2}$ ,  $V = (e_1, \dots, e_r)$ . Then

$$Z_{n+1}^T \Lambda^{1/2} (V V^T - \hat{V} \hat{V}^T) \Lambda^{1/2} Z_{n+1} = o(\sqrt{p}) \quad (36)$$

Lemma 4 is from Wang Rui's paper.

**Lemma 5.** Suppose  $F_n(\cdot)$  and  $F(\cdot)$  are distribution functions and  $F_n \xrightarrow{L} F$ , then

$$\sup_x |F_n(x) - F(x)| \rightarrow 0. \quad (37)$$

See Exercise 3.2.9 of [5].

**Lemma 6.** Suppose  $Z$  is an  $p \times n$  ( $p \geq n$ ) random matrix with all elements i.i.d. distributed as  $N(0, 1)$ . Denote by  $Z = U \Lambda V^T$  the singular value decomposition (SVD) of  $Z$ , where  $U$  is a  $p \times n$  orthogonal matrix,  $\Lambda$  is an  $n \times n$  diagonal matrix and  $V$  is an  $n \times n$  orthogonal matrix. Then  $U$ ,  $\Lambda$  and  $V$  are independent. (See, e.g., [6])

**Lemma 7.** Let  $A$  be an  $n \times n$  symmetric positive semi-definite matrix with rank  $r$ . Denote by  $A = P \Lambda P^T$  the spectral decomposition of  $A$ , where  $P$  is an  $n \times r$  orthogonal matrix and  $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_r)$  is an  $r \times r$  diagonal matrix with  $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_r > 0$ . Then we have

$$(A + I_n)^{-1} \geq I_n - P P^T \quad (38)$$

*Proof.* Let  $\tilde{P}$  be an  $n \times n$  orthogonal matrix such that  $P$  is the first  $r$  columns of  $\tilde{P}$ . And let  $\tilde{\Lambda} = \text{diag}(\lambda_1, \dots, \lambda_r, 0, \dots, 0)$  be an  $n \times n$  matrix. Then  $P \Lambda P^T = \tilde{P} \tilde{\Lambda} \tilde{P}^T$ , and

$$\begin{aligned} (A + I_n)^{-1} &= \tilde{P} (\tilde{\Lambda} + I_n)^{-1} \tilde{P}^T \\ &= \tilde{P} \text{diag}((\lambda_1 + 1)^{-1}, \dots, (\lambda_r + 1)^{-1}, 1, \dots, 1) \tilde{P}^T \\ &\geq \tilde{P} \text{diag}(0, \dots, 0, 1, \dots, 1) \tilde{P}^T \\ &= I_n - P P^T \end{aligned} \quad (39)$$

□

#### 4.2. circumstance 1

##### 4.2.1. First randomization of $\beta$

Independent of data, generate a random  $p$  dimensional orthonormal matrix  $O$  with Haar invariant distribution. And

$$T = \frac{(O\beta)^T O\tilde{X}(O\tilde{X})^T O\beta + 2(O\beta)^T \tilde{X}\tilde{\epsilon} + \tilde{\epsilon}^T \tilde{\epsilon}}{(O\beta)^T O\tilde{X}((O\tilde{X})^T O\tilde{X})^{-1} (O\tilde{X})^T \beta + 2(O\beta)^T O\tilde{X}((O\tilde{X})^T O\tilde{X})^{-1} \tilde{\epsilon} + \tilde{\epsilon}^T ((O\tilde{X})^T O\tilde{X})^{-1} \tilde{\epsilon}} \quad (40)$$

Note that conditioning on  $O$ ,  $O\tilde{X}$  is a random matrix with each entry independently distributed as  $N(0, \lambda)$ . Hence  $O$  is independent of  $O\tilde{X}$ . Observe also that  $O\beta/\|\beta\|$  is uniformly distributed on the unit ball. We can without loss of generality and assume that  $\beta/\|\beta\|$  is uniformly distributed on the surface unit ball in (32).

##### 4.2.2. Second randomization of $\beta$

Independent of data, generate  $R > 0$  with  $R^2$  distributed as  $\chi_p^2$ . Then  $\xi = R\beta/\|\beta\|$  distributed as  $N_p(0, I_p)$ . Note that conditioning on  $\tilde{X}$ ,  $\eta = (\tilde{X}^T \tilde{X})^{-1/2} \tilde{X}^T \xi$  is distributed as  $N_{n-1}(0, I_{n-1})$ . Hence  $\eta$  is independent of  $\tilde{X}$ .

Then

$$\begin{aligned} T &= \frac{(\|\beta\|/R)^2 \xi^T \tilde{X} \tilde{X}^T \xi + 2(\|\beta\|/R) \xi^T \tilde{X} \tilde{\epsilon} + \tilde{\epsilon}^T \tilde{\epsilon}}{(\|\beta\|/R)^2 \xi^T \tilde{X} (\tilde{X}^T \tilde{X})^{-1} \tilde{X}^T \xi + 2(\|\beta\|/R) \xi^T \tilde{X} (\tilde{X}^T \tilde{X})^{-1} \tilde{\epsilon} + \tilde{\epsilon}^T (\tilde{X}^T \tilde{X})^{-1} \tilde{\epsilon}} \\ &= \frac{(\|\beta\|/R)^2 \eta^T \tilde{X}^T \tilde{X} \eta + 2(\|\beta\|/R) \eta^T (\tilde{X}^T \tilde{X})^{1/2} \tilde{\epsilon} + \tilde{\epsilon}^T \tilde{\epsilon}}{(\|\beta\|/R)^2 \eta^T \eta + 2(\|\beta\|/R) \eta^T (\tilde{X}^T \tilde{X})^{-1/2} \tilde{\epsilon} + \tilde{\epsilon}^T (\tilde{X}^T \tilde{X})^{-1} \tilde{\epsilon}} \\ &= \frac{A_1 + A_2 + A_3}{B_1 + B_2 + B_3} \end{aligned} \quad (41)$$

#### 4.2.3. Step 3: CLT

Similar to the derivation of the distribution of Hotelling's  $T^2$  statistic.

Now we deal with

$$\frac{A_3}{B_3} = \frac{\tilde{\epsilon}^T \tilde{\epsilon}}{\tilde{\epsilon}^T (\tilde{X}^T \tilde{X})^{-1} \tilde{\epsilon}} \quad (42)$$

Let  $O$  be an  $(n-1) \times (n-1)$  orthogonal matrix satisfies

$$O\tilde{\epsilon} = \begin{pmatrix} \|\tilde{\epsilon}\| \\ 0 \\ \dots \\ 0 \end{pmatrix}.$$

Then

$$\frac{A_3}{B_3} = \frac{(O\tilde{\epsilon})^T O\tilde{\epsilon}}{(O\tilde{\epsilon})^T ((\tilde{X}O^T)^T \tilde{X}O^T)^{-1} O\tilde{\epsilon}}. \quad (43)$$

It can be seen that  $\tilde{X}O^T$  has the same distribution as  $\tilde{X}$  and is independent of  $O$ . We have

$$\frac{A_3}{B_3} \sim \frac{1}{((\tilde{X}^T \tilde{X})^{-1})_{11}}. \quad (44)$$

Apply Lemma 1, we have

$$\frac{A_3}{B_3} \sim (\tilde{X}^T \tilde{X})_{11 \cdot 2}. \quad (45)$$

Since  $\tilde{X}^T \tilde{X} \sim \text{Wishart}_{n-1}(\lambda I_{n-1}, p)$ ,  $(\tilde{X}^T \tilde{X})_{11 \cdot 2} \sim \lambda \chi_{p-n+2}^2$ . Hence  $A_3/B_3 \asymp p$  and

$$\frac{A_3/B_3 - \lambda(p-n+2)}{\lambda\sqrt{2(p-n+2)}} \xrightarrow{\mathcal{L}} N(0, 1), \quad (46)$$

by CLT.

Similar technique can deal with  $A_1/B_1$ :

$$\frac{A_1}{B_1} = \frac{\eta^T \tilde{X}^T \tilde{X} \eta}{\eta^T \eta} \sim (\tilde{X}^T \tilde{X})_{11} \sim \lambda \chi_p^2. \quad (47)$$

Hence  $A_1/B_1 \asymp p$  and

$$\frac{A_1/B_1 - \lambda p}{\lambda\sqrt{2p}} \xrightarrow{\mathcal{L}} N(0, 1), \quad (48)$$

by CLT.

4.2.4. *step 4*

It's obvious that  $A_3 \asymp n$  and  $B_1 \asymp \frac{n}{p} \|\beta\|^2$ . We already have  $A_1/B_1 \asymp p$  and  $A_3/B_3 \asymp p$ . It follows that  $A_1 \asymp n \|\beta\|^2$  and  $B_3 \asymp n/p$ . And

$$\begin{aligned}
A_2 &= O_P(\|\beta\|/\sqrt{p}) \eta^T (\tilde{X}^T \tilde{X})^{1/2} \tilde{\epsilon} \\
&= O_P(\|\beta\|/\sqrt{p}) \sqrt{\eta^T (\tilde{X}^T \tilde{X}) \eta} \\
&= O_P(\|\beta\|/\sqrt{p}) O_P(\sqrt{np}) \\
&= O_P(\sqrt{n} \|\beta\|),
\end{aligned} \tag{49}$$

$$\begin{aligned}
B_2 &= O_P(\|\beta\|/\sqrt{p}) \eta^T (\tilde{X}^T \tilde{X})^{-1/2} \tilde{\epsilon} \\
&= O_P(\|\beta\|/\sqrt{p}) \sqrt{\eta^T (\tilde{X}^T \tilde{X})^{-1} \eta} \\
&= O_P(\|\beta\|/\sqrt{p}) O_P(\sqrt{n/p}) \\
&= O_P\left(\frac{\sqrt{n}}{p} \|\beta\|\right).
\end{aligned} \tag{50}$$

Note that

$$A_2 = O_P\left(\frac{1}{\sqrt{n}}\right) n \|\beta\| = O_P\left(\frac{1}{\sqrt{n}}\right) \sqrt{A_1} \sqrt{A_3} \leq O_P\left(\frac{1}{\sqrt{n}}\right) (A_1 + A_3) \tag{51}$$

Similarly we have  $B_2 = O_P\left(\frac{1}{\sqrt{n}}\right) (B_1 + B_3)$ . It follows that

$$T = \frac{A_1 + A_3}{B_1 + B_3} (1 + O_P\left(\frac{1}{\sqrt{n}}\right)). \tag{52}$$

For every  $\epsilon > 0$ , we have

$$\begin{aligned}
&\Pr\left(\frac{A_1 + A_3}{B_1 + B_3} \geq (\lambda p)(1 + \epsilon)\right) \\
&= \Pr(A_1 + A_3 \geq (B_1 + B_3)(\lambda p)(1 + \epsilon)) \\
&\leq \Pr(A_1 \geq B_1(\lambda p)(1 + \epsilon)) + \Pr(A_3 \geq B_3(\lambda p)(1 + \epsilon)).
\end{aligned} \tag{53}$$

But

$$\frac{A_1}{\lambda p B_1} \xrightarrow{P} 1 \quad \text{and} \quad \frac{A_3}{\lambda p B_3} \xrightarrow{P} 1. \tag{54}$$

It follows that (53) tends to 0. Similarly,

$$\Pr\left(\frac{A_1 + A_3}{B_1 + B_3} \leq (\lambda p)(1 - \epsilon)\right) \rightarrow 0. \tag{55}$$

We have proved

$$\frac{A_1 + A_3}{\lambda p(B_1 + B_3)} \xrightarrow{P} 1. \quad (56)$$

Together with (52), it follows that  $T \xrightarrow{P} 1$ .

#### 4.2.5. Step 5

By Cauchy inequality,  $\tilde{\epsilon}^T(\tilde{X}^T \tilde{X})^{-1} \tilde{\epsilon} \tilde{\epsilon}^T \tilde{X}^T \tilde{X} \tilde{\epsilon} \geq (\tilde{\epsilon}^T \tilde{\epsilon})^2$ . Denote  $B_4 = \tilde{\epsilon}^T \tilde{X}^T \tilde{X} \tilde{\epsilon}$ . Using similar technique as before, we have  $B_4 \asymp np$  and  $(B_4/A_3 - \lambda p)/(\lambda\sqrt{2p}) \xrightarrow{\mathcal{L}} N(0, 1)$ . Together with (52) and (56), we have

$$\begin{aligned} T &= \frac{A_1 + A_3}{B_1 + B_3} \frac{1 + \frac{A_2}{A_1 + A_3}}{1 + \frac{B_2}{B_1 + B_3}} \\ &= \frac{A_1 + A_3}{B_1 + B_3} \left(1 + \frac{A_2}{A_1 + A_3}\right) \left(1 - \frac{B_2}{B_1 + B_3} (1 + o_P(1))\right) \\ &= \frac{A_1 + A_3}{B_1 + B_3} \left(1 + \left(\frac{|A_2|}{A_1 + A_3} + \frac{|B_2|}{B_1 + B_3}\right) (1 + o_P(1))\right) \\ &= \frac{A_1 + A_3}{B_1 + B_3} + O_P(p) \left(\frac{|A_2|}{A_1 + A_3} + \frac{|B_2|}{B_1 + B_3}\right) \\ &= \frac{A_1 + A_3}{B_1 + B_3} + O_P(p) \left(\frac{\sqrt{n}\|\beta\|}{n\|\beta\|^2 + n} + \frac{\frac{\sqrt{n}}{p}\|\beta\|}{\frac{n}{p}\|\beta\|^2 + \frac{n}{p}}\right) \\ &= \frac{A_1 + A_3}{B_1 + B_3} + O_P\left(\frac{p\sqrt{n}\|\beta\|}{n\|\beta\|^2 + n}\right) \\ &\leq \frac{A_1 + A_3}{B_1 + A_3^2/B_4} + O_P\left(\frac{p\sqrt{n}\|\beta\|}{n\|\beta\|^2 + n}\right). \end{aligned} \quad (57)$$

We deal with the two terms separately.

$$\frac{\frac{A_1 + A_3}{B_1 + A_3^2/B_4} - \lambda p}{\lambda\sqrt{2p}} = c \frac{A_1/B_1 - \lambda p}{\lambda\sqrt{2p}} + (1 - c) \frac{B_4/A_3 - \lambda p}{\lambda\sqrt{2p}}, \quad (58)$$

where

$$c = \frac{B_1}{B_1 + A_3^2/B_4} \asymp \frac{\frac{n}{p}\|\beta\|^2}{\frac{n}{p}\|\beta\|^2 + \frac{n}{p}} = \frac{\|\beta\|^2}{\|\beta\|^2 + 1}. \quad (59)$$

Hence by Slutsky's theorem, we have

$$\frac{\frac{A_1 + A_3}{B_1 + A_3^2/B_4} - \lambda p}{\lambda\sqrt{2p}} \xrightarrow{\mathcal{L}} N(0, 1), \quad (60)$$

if  $\|\beta\| \rightarrow 0$  or  $\|\beta\| \rightarrow \infty$ .

To control the second term of (57), we further require

$$\frac{\sqrt{np}\|\beta\|}{n\|\beta\|^2 + n} \rightarrow 0. \quad (61)$$

Equivalently, if  $\|\beta\| \rightarrow 0$ , we require  $\|\beta\| = o(\frac{\sqrt{n}}{\sqrt{p}})$ ; if  $\|\beta\| \rightarrow \infty$ , we require  $\|\beta\|^{-1} = o(\frac{\sqrt{n}}{\sqrt{p}})$ .

If these conditions are satiesfied, we have

$$\Pr\left(\frac{T - \lambda p}{\lambda\sqrt{2p}} \geq \Phi^{-1}(1 - \alpha)\right) \leq \alpha \quad (62)$$

#### 4.3. circumstance 2

**Assumption 3.**  $P_1^T \beta = 0$ .

$$\begin{aligned} T &= \frac{\beta^T \tilde{X} \tilde{X}^T \beta + 2\beta^T \tilde{X} \tilde{\epsilon} + \tilde{\epsilon}^T \tilde{\epsilon}}{\beta^T \tilde{X} (\tilde{X}^T \tilde{X})^{-1} \tilde{X}^T \beta + 2\beta^T \tilde{X} (\tilde{X}^T \tilde{X})^{-1} \tilde{\epsilon} + \tilde{\epsilon}^T (\tilde{X}^T \tilde{X})^{-1} \tilde{\epsilon}} \\ &= \frac{\beta^T P_2 P_2^T \tilde{X} \tilde{X}^T P_2 P_2^T \beta + 2\beta^T P_2 P_2^T \tilde{X} \tilde{\epsilon} + \tilde{\epsilon}^T \tilde{\epsilon}}{\beta^T P_2 P_2^T \tilde{X} (\tilde{X}^T \tilde{X})^{-1} \tilde{X}^T P_2 P_2^T \beta + 2\beta^T P_2 P_2^T \tilde{X} (\tilde{X}^T \tilde{X})^{-1} \tilde{\epsilon} + \tilde{\epsilon}^T (\tilde{X}^T \tilde{X})^{-1} \tilde{\epsilon}} \\ &= \frac{A_1 + A_2 + A_3}{B_1 + B_2 + B_3} \end{aligned} \quad (63)$$

##### 4.3.1. Step 1

Like before, we have  $A_3/B_3 \sim (\tilde{X}^T \tilde{X})_{11,2}$ . Denote by  $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_p)$ . Let  $Z = (Z_1, \dots, Z_p)$  be a  $n - 1 \times p$  matrix with all elements independently distributed as  $N(0, 1)$ . Let  $Z_{(1)}$  and  $Z_{(2)}$  be the first 1 row and last  $n - 2$  rows of  $Z$ , that is

$$Z = \begin{pmatrix} Z_{(1)} \\ Z_{(2)} \end{pmatrix}.$$

Then

$$\begin{aligned} \tilde{X}^T \tilde{X} &\sim Z \Lambda Z^T \\ &= \begin{pmatrix} Z_{(1)} \Lambda Z_{(1)}^T & Z_{(1)} \Lambda Z_{(2)}^T \\ Z_{(2)} \Lambda Z_{(1)}^T & Z_{(2)} \Lambda Z_{(2)}^T \end{pmatrix}. \end{aligned} \quad (64)$$

Hence

$$\begin{aligned}
A_3/B_3 &\sim Z_{(1)}\Lambda Z_{(1)}^T - Z_{(1)}\Lambda Z_{(2)}^T(Z_{(2)}\Lambda Z_{(2)}^T)^{-1}Z_{(2)}\Lambda Z_{(1)}^T \\
&= Z_{(1)}\Lambda^{1/2}(I_p - \Lambda^{1/2}Z_{(2)}^T(Z_{(2)}\Lambda Z_{(2)}^T)^{-1}Z_{(2)}\Lambda^{1/2})\Lambda^{1/2}Z_{(1)}^T \quad (65) \\
&\leq Z_{(1)}\Lambda^{1/2}(I_p - \hat{V}\hat{V}^T)\Lambda^{1/2}Z_{(1)}^T,
\end{aligned}$$

where  $\hat{V}$  is the first  $r$  eigenvectors of  $\Lambda^{1/2}Z_{(2)}^TZ_{(2)}\Lambda^{1/2}$ . From PCA theory (see [1]),  $\hat{V}\hat{V}^T$  is a good estimator of population principal space  $VV^T$  even in high dimensional setting. Here  $V = (e_1, \dots, e_r)$ , where  $e_i$  is the vector with all elements equal to 0 but the  $i$ th equal to 1. Note that we have required  $p = o(n^2)$ . Then by lemma 4,

$$Z_{(1)}\Lambda^{1/2}(VV^T - \hat{V}\hat{V}^T)\Lambda^{1/2}Z_{(1)}^T = o(\sqrt{p}). \quad (66)$$

Note that

$$Z_{(1)}\Lambda^{1/2}(I - VV^T)\Lambda^{1/2}Z_{(1)}^T \sim \lambda\chi_{p-r}^2 \quad (67)$$

Hence  $A_3/B_3 \leq \lambda\chi_{p-r}^2 + o(\sqrt{p})$ .

On the other hand, the non-zero eigenvalues of  $\Lambda^{1/2}(I_p - \Lambda^{1/2}Z_{(2)}^T(Z_{(2)}\Lambda Z_{(2)}^T)^{-1}Z_{(2)}\Lambda^{1/2})\Lambda^{1/2}$  is no less than that of  $\lambda(I_p - \Lambda^{1/2}Z_{(2)}^T(Z_{(2)}\Lambda Z_{(2)}^T)^{-1}Z_{(2)}\Lambda^{1/2})$ . Hence  $A_3/B_3 \geq \lambda\chi_{p-n+2}^2$ .

It follows that  $A_3/B_3 \asymp p$  if  $p/n \rightarrow \infty$ .

#### 4.3.2. Step 2: $B_1$ and $B_2$

Note that  $P_2^T\tilde{X}$  is an  $(p-r) \times (n-1)$  matrix with all elements independently distributed as  $N(0, \lambda)$ . Similar to non-spiked circumstance, we have  $A_1 \asymp n\|P_2^T\beta\|^2$ ,  $A_2 = O_P(\sqrt{n}\|P_2^T\beta\|)$ ,  $A_3 \asymp n$  and  $B_3 \asymp n/p$ .

Next we deal with  $B_1$ . Let  $P_2^T\tilde{X} = U_2D_2V_2^T$  be the SVD of  $P_2^T\tilde{X}$ , where  $U_2$  is a  $(p-r) \times (n-1)$  orthonormal matrix,  $D_2$  is a  $(n-1) \times (n-1)$  diagonal matrix and  $V_2$  is a  $(n-1) \times (n-1)$  orthonormal matrix. Without loss of generality, we can assume  $P_2^T\beta/\|P_2^T\beta\|$  is uniformly distributed on the surface of unit ball.

$B_1$  has the following upper bound:

$$\begin{aligned} B_1 &\leq \beta^T P_2 P_2^T \tilde{X} (\tilde{X}^T P_2 P_2^T \tilde{X})^{-1} \tilde{X}^T P_2 P_2^T \beta \\ &= \beta^T P_2 U_2 U_2^T P_2^T \beta \end{aligned} \quad (68)$$

Independent of  $P_2^T \beta / \|P_2^T \beta\|$  and  $U_2$ , we generate  $R \sim \chi_{p-r}^2$ . Then we have

$$\sqrt{R} \frac{P_2^T \beta}{\|P_2^T \beta\|} \sim N_{p-r}(0, I_{p-r}). \quad (69)$$

Hence

$$\begin{aligned} &\beta^T P_2 U_2 U_2^T P_2^T \beta \\ &= \frac{\sqrt{R} \beta^T P_2}{\|P_2 \beta\|} U_2 U_2^T \frac{\sqrt{R} P_2^T \beta}{\|P_2^T \beta\|} \frac{1}{R} \|P_2^T \beta\|^2 \\ &\asymp \frac{n-1}{p-r} \|P_2^T \beta\|^2. \end{aligned} \quad (70)$$

To get the lower bound, note that

$$\begin{aligned} B_1 &= \beta^T P_2 P_2^T \tilde{X} (\tilde{X}^T P_1 P_1^T \tilde{X} + \tilde{X}^T P_2 P_2^T \tilde{X})^{-1} \tilde{X}^T P_2 P_2^T \beta \\ &= \beta^T P_2 U_2 D_2 V_2^T (\tilde{X}^T P_1 P_1^T \tilde{X} + V_2 D_2^2 V_2^T)^{-1} V_2 D_2 U_2^T P_2^T \beta \\ &= \beta^T P_2 U_2 (D_2^{-1} V_2^T \tilde{X}^T P_1 P_1^T \tilde{X} V_2 D_2^{-1} + I_{n-1})^{-1} U_2^T P_2^T \beta. \end{aligned} \quad (71)$$

Here  $U_2$  is independent of  $(V_2, D_2, P_1^T \tilde{X})$ . By lemma 7

$$(D_2^{-1} V_2^T \tilde{X}^T P_1 P_1^T \tilde{X} V_2 D_2^{-1} + I_{n-1})^{-1} \geq I_{n-1} - U^* U^{*T} \quad (72)$$

where  $U^*$  is the first  $r$  eigenvectors of  $D_2^{-1} V_2^T \tilde{X}^T P_1 P_1^T \tilde{X} V_2 D_2^{-1}$  and is independent of  $U_2$ . Since  $U_2$  has Haar distribution, we have

$$\begin{aligned} B_1 &\geq \beta^T P_2 U_2 (I_{n-1} - U^* U^{*T}) U_2^T P_2^T \beta \\ &= \beta^T P_2 U_2 U_2^T P_2^T \beta - \beta^T P_2 U_2 U^* U^{*T} U_2^T P_2^T \beta. \end{aligned} \quad (73)$$

The difference of upper bound and lower bound is

$$\beta^T P_2 U_2 U^* U^{*T} U_2^T P_2^T \beta \asymp \frac{r}{p-r} \|P_2^T \beta\|^2. \quad (74)$$

Hence

$$\begin{aligned} B_1 &= \beta^T P_2 P_2^T \tilde{X} (\tilde{X}^T P_2 P_2^T \tilde{X})^{-1} \tilde{X}^T P_2 P_2^T \beta + O_p\left(\frac{r}{p-r} \|P_2^T \beta\|^2\right) \\ &= \beta^T P_2 P_2^T \tilde{X} (\tilde{X}^T P_2 P_2^T \tilde{X})^{-1} \tilde{X}^T P_2 P_2^T \beta (1 + O_P(1/n)). \end{aligned} \quad (75)$$



So that  $B_1 \asymp \frac{n}{p} \|P_2^T \beta\|^2$ .

For  $B_2$  we have

$$\begin{aligned} B_2 &= O_P(1) \sqrt{\beta^T P_2 P_2^T \tilde{X} (\tilde{X}^T \tilde{X})^{-2} \tilde{X}^T P_2 P_2^T \beta} \\ &\leq \lambda_{\min}(\tilde{X}^T \tilde{X})^{-1/2} O_P(1) \sqrt{\beta^T P_2 P_2^T \tilde{X} (\tilde{X}^T \tilde{X})^{-1} \tilde{X}^T P_2 P_2^T \beta}. \end{aligned} \quad (76)$$

But  $\lambda_{\min}(\tilde{X}^T \tilde{X}) \geq \lambda_{\min}(\tilde{X}^T P_2 P_2^T \tilde{X}) \asymp p - r$  by Lemma 3. Hence  $B_2 = O_P(\frac{\sqrt{n}}{p} \|P_2^T \beta\|)$ .

Hence the similar law of large number and CLT holds.

#### 4.3.3. Step 3

Use similar technique as before, we have

$$\frac{A_1}{B_1} \sim \frac{\chi_p^2}{1 + O_P(1/n)} = \lambda \chi_p^2 (1 + O_P(1/n)). \quad (77)$$

It follows by large number that

$$\frac{A_1/B_1}{\lambda p} \xrightarrow{P} 1. \quad (78)$$

And if  $p = o(n^2)$ , we have

$$\frac{A_1/B_1 - \lambda p}{\lambda \sqrt{2p}} \sim \frac{\chi_p^2 (1 + O_P(1/n)) - p}{\sqrt{2p}} \xrightarrow{\mathcal{L}} N(0, 1). \quad (79)$$

Recall that if  $p = o(n^2)$ , we have  $A_3/B_3 \geq \lambda \chi_{p-n+2}^2$  and  $A_3/B_3 \leq \lambda \chi_{p-r}^2 + o(\sqrt{p}) \leq \lambda \chi_p^2 + o(\sqrt{p})$ . Then

$$\frac{A_3/B_3}{\lambda p} \xrightarrow{P} 1, \quad (80)$$

and

$$\frac{A_3/B_3 - \lambda p}{\lambda \sqrt{2p}} \leq \frac{\chi_p^2 + o(\sqrt{p}) - p}{\sqrt{2p}} \xrightarrow{\mathcal{L}} N(0, 1). \quad (81)$$

From (78) and (80) we can deduce  $T/(\lambda p) \xrightarrow{P} 1$  by similar argument as before.

Similar to (57), we have

$$T \leq \frac{A_1 + A_3}{B_1 + A_3} + O_P\left(\frac{p\sqrt{n}\|P_2^T \beta\|}{n\|P_2^T \beta\|^2 + n}\right). \quad (82)$$

For the first term, we have

$$\frac{\frac{A_1+A_3}{B_1+B_3} - \lambda p}{\lambda\sqrt{2p}} = c \frac{\frac{A_1}{B_1} - \lambda p}{\lambda\sqrt{2p}} + (1-c) \frac{\frac{A_3}{B_3} - \lambda p}{\lambda\sqrt{2p}}, \quad (83)$$

where

$$c = \frac{B_1}{B_1+B_3} \asymp \frac{\|P_2^T \beta\|^2}{\|P_2^T \beta\|^2 + 1}. \quad (84)$$

Then theorem follows by the same argument as before.

#### 4.4. Consistency of Test

Since  $\beta \sim N(0, \sigma_\beta^2 I_p)$  and  $(\tilde{X}^T \tilde{X})^{-1/2} \tilde{X}^T$  is a projection matrix, we have  $\gamma = (\tilde{X}^T \tilde{X})^{-1/2} \tilde{X}^T \beta \sim N(0, \sigma_\beta^2 I_{n-1})$ . Then

$$\begin{aligned} T &= \frac{\beta^T \tilde{X} \tilde{X}^T \beta + 2\beta^T \tilde{X} \tilde{\epsilon} + \tilde{\epsilon}^T \tilde{\epsilon}}{\beta^T \tilde{X} (\tilde{X}^T \tilde{X})^{-1} \tilde{X}^T \beta + 2\beta^T \tilde{X} (\tilde{X}^T \tilde{X})^{-1} \tilde{\epsilon} + \tilde{\epsilon}^T (\tilde{X}^T \tilde{X})^{-1} \tilde{\epsilon}} \\ &= \frac{\gamma^T \tilde{X}^T \tilde{X} \gamma + 2\gamma^T (\tilde{X}^T \tilde{X})^{1/2} \tilde{\epsilon} + \tilde{\epsilon}^T \tilde{\epsilon}}{\gamma^T \gamma + 2\gamma^T (\tilde{X}^T \tilde{X})^{-1/2} \tilde{\epsilon} + \tilde{\epsilon}^T (\tilde{X}^T \tilde{X})^{-1} \tilde{\epsilon}} \\ &= \frac{A_1 + A_2 + A_3}{B_1 + B_2 + B_3}. \end{aligned} \quad (85)$$

It can be seen that  $A_1 \sim \|\gamma\|^2 \sum_{i=1}^p \lambda_i \chi_1^2 \asymp \|\gamma\|^2 (p + \lambda_1) \asymp \sigma_\beta^2 n(p + \lambda_1)$ ,  $A_2 = O_P(\sqrt{A_1})$  and  $A_3 \asymp n$ . As for the denominator of  $T$ , we have  $B_1 \asymp \sigma_\beta^2 n$ ,  $B_3 \leq \tilde{\epsilon}^T (\tilde{X}^T P_2 P_2^T \tilde{X})^{-1} \tilde{\epsilon} \asymp n/p$  and  $B_2 = O_P(\sqrt{B_3} \sigma_\beta)$ .

By similar technique as before, we have  $A_1/B_1 \sim \sum_{i=1}^p \lambda_i \chi_1^2$ . By CLT and Slutsky's theorem, we have

$$\frac{\sum_{i=r+1}^p \lambda_i \chi_1^2 - p\lambda}{\lambda\sqrt{2p}} \xrightarrow{\mathcal{L}} N(0, 1). \quad (86)$$

And note that if  $p\sigma_\beta^2 \rightarrow \infty$ ,

$$\begin{aligned}
& \left| \frac{T - \lambda p}{\lambda\sqrt{2p}} - \frac{A_1/B_1 - \lambda p}{\lambda\sqrt{2p}} \right| \\
&= \frac{1}{\lambda\sqrt{2p}} \left| \frac{A_1 + A_2 + A_3}{B_1 + B_2 + B_3} - \frac{A_1}{B_1} \right| \\
&= \frac{1}{\lambda\sqrt{2p}} \left| \frac{(A_2 + A_3)B_1 - (B_2 + B_3)A_1}{(B_1 + B_2 + B_3)B_1} \right| \\
&= \frac{O_P(1)}{\lambda\sqrt{2p}} \left| \frac{(O_P(\sigma_\beta\sqrt{n(p+\lambda_1)}) + O_P(n))O_P(\sigma_\beta^2 n) - (O_P(\sigma_\beta\frac{\sqrt{n}}{\sqrt{p}}) + O_P(\frac{n}{p}))O_P(\sigma_\beta^2 n(p+\lambda_1))}{\sigma_\beta^4 n^2} \right| \\
&= O_P\left(\frac{p+\lambda_1}{\sigma_\beta\sqrt{np}}\right) + O_P\left(\frac{p+\lambda_1}{\sigma_\beta^2 p^{3/2}}\right).
\end{aligned} \tag{87}$$

Hence if

$$\frac{np^2 + p^{5/2} + \lambda_1 p^{3/2}}{(p + \lambda_1)^2} \sigma_\beta^2 \rightarrow \infty, \tag{88}$$

then

$$\left| \frac{T - \lambda p}{\lambda\sqrt{2p}} - \frac{A_1/B_1 - \lambda p}{\lambda\sqrt{2p}} \right| = o_P(1). \tag{89}$$

Equivalently, there exists a positive sequence  $\epsilon_n \rightarrow 0$  such that

$$\Pr\left(\left| \frac{T - \lambda p}{\lambda\sqrt{2p}} - \frac{A_1/B_1 - \lambda p}{\lambda\sqrt{2p}} \right| > \epsilon_n\right) < \epsilon_n. \tag{90}$$

Then it follows by Lemma 5 and Slutsky's theorem that

$$\begin{aligned}
& \Pr\left(\frac{T - p\lambda}{\lambda\sqrt{2p}} \geq \Phi^{-1}(1 - \alpha)\right) \\
&= \Pr\left(\frac{T - p\lambda}{\lambda\sqrt{2p}} \geq \Phi^{-1}(1 - \alpha), \left| \frac{T - \lambda p}{\lambda\sqrt{2p}} - \frac{A_1/B_1 - \lambda p}{\lambda\sqrt{2p}} \right| \leq \epsilon_n\right) + o(1) \\
&\geq \Pr\left(\frac{A_1/B_1 - p\lambda}{\lambda\sqrt{2p}} - \epsilon_n \geq \Phi^{-1}(1 - \alpha), \left| \frac{T - \lambda p}{\lambda\sqrt{2p}} - \frac{A_1/B_1 - \lambda p}{\lambda\sqrt{2p}} \right| \leq \epsilon_n\right) + o(1) \\
&= \Pr\left(\frac{A_1/B_1 - p\lambda}{\lambda\sqrt{2p}} - \epsilon_n \geq \Phi^{-1}(1 - \alpha)\right) + o(1) \\
&= \mathbb{E} \Pr\left(\frac{\sum_{i=r+1}^p \lambda_i \chi_i^2 - p\lambda}{\lambda\sqrt{2p}} - \epsilon_n \geq \Phi^{-1}(1 - \alpha) - \frac{\sum_{i=1}^r \lambda_i \chi_i^2}{\lambda\sqrt{2p}} \middle| \sum_{i=1}^r \lambda_i \chi_i^2\right) + o(1) \\
&= \mathbb{E} \Phi\left(-\Phi^{-1}(1 - \alpha) + \frac{\sum_{i=1}^r \lambda_i \chi_i^2}{\lambda\sqrt{2p}}\right) + o(1).
\end{aligned} \tag{91}$$

Similarly we get the lower bound. Then

$$\Pr\left(\frac{T - p\lambda}{\lambda\sqrt{2p}} \geq \Phi^{-1}(1 - \alpha)\right) = \mathbb{E}\Phi\left(-\Phi^{-1}(1 - \alpha) + \frac{\sum_{i=1}^r \lambda_i \chi_i^2}{\lambda\sqrt{2p}}\right) + o(1). \quad (92)$$

4.5.  $\hat{\lambda}$

Note that  $\tilde{X}^T \tilde{X} = \tilde{X}^T P_1 P_1^T \tilde{X} + \tilde{X}^T P_2 P_2^T \tilde{X}$ . By Lemma 2, we have

$$\lambda_i(\tilde{X}^T P_2 P_2^T \tilde{X}) \leq \lambda_i(\tilde{X}^T \tilde{X}) \leq \lambda_{r+1}(\tilde{X}^T P_1 P_1^T \tilde{X}) + \lambda_{i-r}(\tilde{X}^T P_2 P_2^T \tilde{X}), \quad (93)$$

for  $i \geq r + 1$ . Note that  $\lambda_{r+1}(\tilde{X}^T P_1 P_1^T \tilde{X}) = 0$  since the rank of  $\tilde{X}^T P_1 P_1^T \tilde{X}$  is  $r$ . Sum the above inequality from  $i = k + 1$  to  $n - 1$  and we obtain

$$\sum_{i=k+1}^{n-1} \lambda_i(\tilde{X}^T P_2 P_2^T \tilde{X}) \leq \sum_{i=k+1}^{n-1} \lambda_i(\tilde{X}^T \tilde{X}) \leq \sum_{i=k-r+1}^{n-r-1} \lambda_i(\tilde{X}^T P_2 P_2^T \tilde{X}). \quad (94)$$

Hence by Lemma 3,

$$\left| \sum_{i=k+1}^{n-1} \lambda_i(\tilde{X}^T \tilde{X}) - \sum_{i=1}^{n-1} \lambda_i(\tilde{X}^T P_2 P_2^T \tilde{X}) \right| \leq k \lambda_1(\tilde{X}^T P_2 P_2^T \tilde{X}) = O_P(p). \quad (95)$$

Since

$$\sum_{i=1}^{n-1} \lambda_i(\tilde{X}^T P_2 P_2^T \tilde{X}) = \text{tr} \tilde{X}^T P_2 P_2^T \tilde{X} \sim \lambda \chi_{(p-k)(n-1)}^2, \quad (96)$$

we have by CLT that

$$\sum_{i=1}^{n-1} \lambda_i(\tilde{X}^T P_2 P_2^T \tilde{X}) = \lambda(p - k)(n - 1) \left(1 + O_P\left(\frac{1}{\sqrt{(p - r)(n - 1)}}\right)\right). \quad (97)$$

It follows from (95) and (97) that

$$\frac{1}{(p - r)(n - 1)} \sum_{i=k+1}^{n-1} \lambda_i(\tilde{X}^T \tilde{X}) = \lambda + O_P\left(\frac{1}{\sqrt{np}}\right) + O_P\left(\frac{1}{n}\right) = \lambda + O_P\left(\frac{1}{n}\right). \quad (98)$$

When  $\lambda$  is substituted by  $\hat{\lambda}$ , the conclusion of Theorem 1, 2 and 3 will be still valid if we can prove

$$\left| \frac{T - \hat{\lambda}p}{\hat{\lambda}\sqrt{2p}} - \frac{T - \lambda p}{\lambda\sqrt{2p}} \right| \xrightarrow{P} 0. \quad (99)$$

In fact

$$\left| \frac{T - \hat{\lambda}p}{\hat{\lambda}\sqrt{2p}} - \frac{T - \lambda p}{\lambda\sqrt{2p}} \right| = \frac{T}{\sqrt{2p}} \frac{|\hat{\lambda} - \lambda|}{\hat{\lambda}\lambda} = O_P\left(\frac{T}{n\sqrt{p}}\right). \quad (100)$$

In Theorem 1 and 2,  $T = O_P(p)$ . Combined with  $p = o(n^2)$ , it follows that (100)  $\xrightarrow{P} 0$ .

In Theorem 3,  $T = O_P(p + \lambda_1)$ . To make (100)  $\xrightarrow{P} 0$ , we require  $(p + \lambda_1)/(n\sqrt{p}) \rightarrow 0$ .

## 5. Simulation Results

### References

- [1] T. T. Cai, Z. Ma, Y. Wu, Sparse pca: Optimal rates and adaptive estimation, *Annals of Statistics* 41 (6) (2012) 3074–3110.
- [2] J. Zhao, X. Xu, A generalized likelihood ratio test for normal mean when p is greater than n, *Computational Statistics & Data Analysis*.
- [3] S. C. Ahn, A. R. Horenstein, Eigenvalue ratio test for the number of factors, *Econometrica* 81 (3) (2013) 1203–1227.  
URL <http://dx.doi.org/10.3982/ECTA8968>
- [4] Z. D. Bai, Y. Q. Yin, Limit of the smallest eigenvalue of a large dimensional sample covariance matrix, *Annals of Probability* 21 (3) (1993) 1275–1294.
- [5] R. Durrett, Probability : theory and examples, *Journal of the American Statistical Association* 87 (418) (2010) 586.
- [6] M. L. Eaton, Multivariate statistics: A vector space approach 80 (392) (1983) 72.